Center for
Electronic Correlations and Magnetism
University of Augsburg

Theory of correlated fermionic condensed matter

1. Correlated electrons made simple

b. Introduction to dynamical mean-field theory (DMFT)

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 5, 2009

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Outline:

- Construction of mean-field theories
- Dynamical mean-field theory (DMFT) for correlated electrons: General conceps

What is a "mean-field theory (MFT)" ?

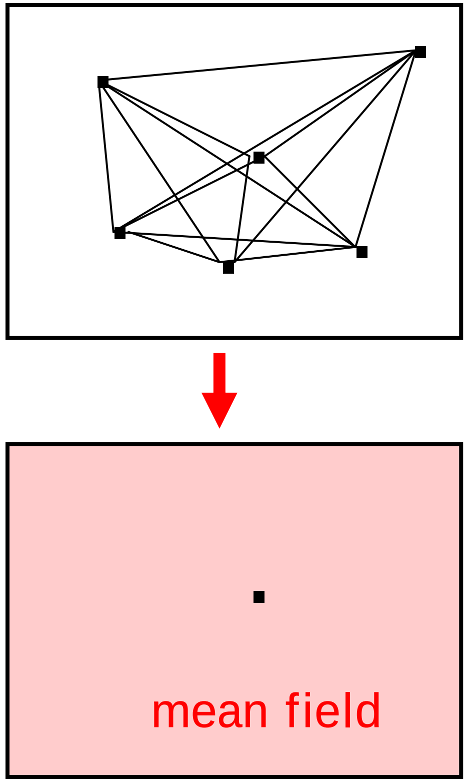
In general: construction by factorization

$$\langle AB \rangle \rightarrow \langle A \rangle \langle B \rangle$$

e.g., spins:

$$\langle S_i S_j \rangle \rightarrow \langle S_i \rangle \langle S_j \rangle$$

→ Weiss MFT



Construction of mean-field theories:

lattice coordination number $Z \to \infty$

or

spatial dimension $d \to \infty$

Interacting spins/particles on a lattice

Hypercubic lattices: Coordination number Z=2d

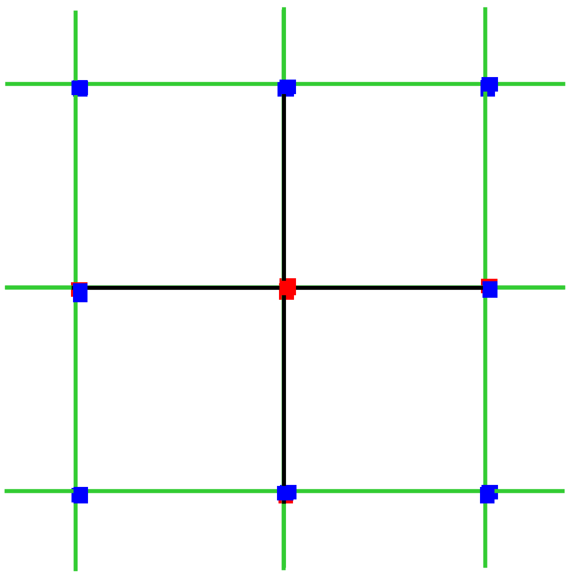
Dimension d=1

Z=2

Interacting spins/particles on a lattice

Hypercubic lattices: Coordination number Z=2d

Dimension d=2

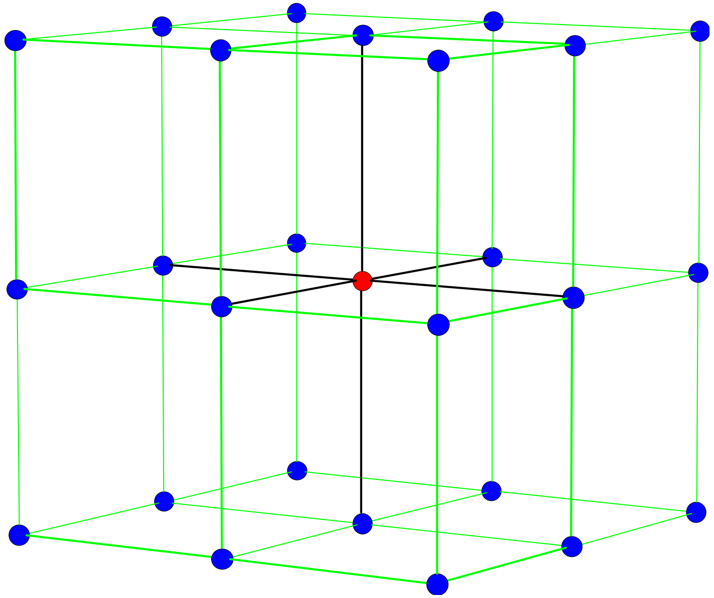


Z=4

Interacting spins/particles on a lattice

Hypercubic lattices: Coordination number Z=2d

Dimension d=3

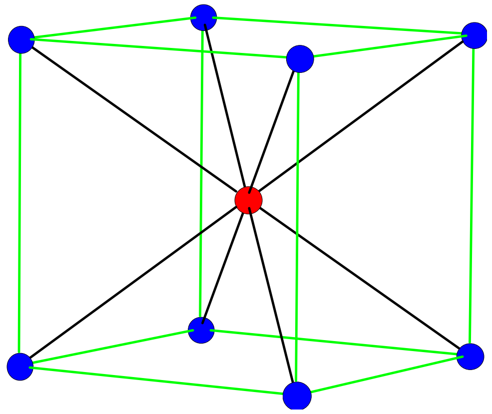


Z=6

Interacting spins/particles on a lattice

Body-centered cubic lattice

Dimension d=3

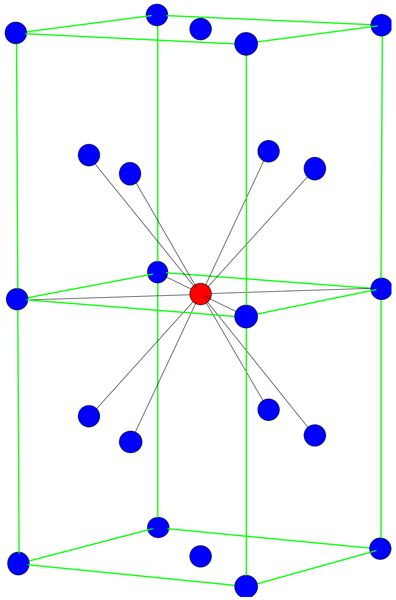


Z=8

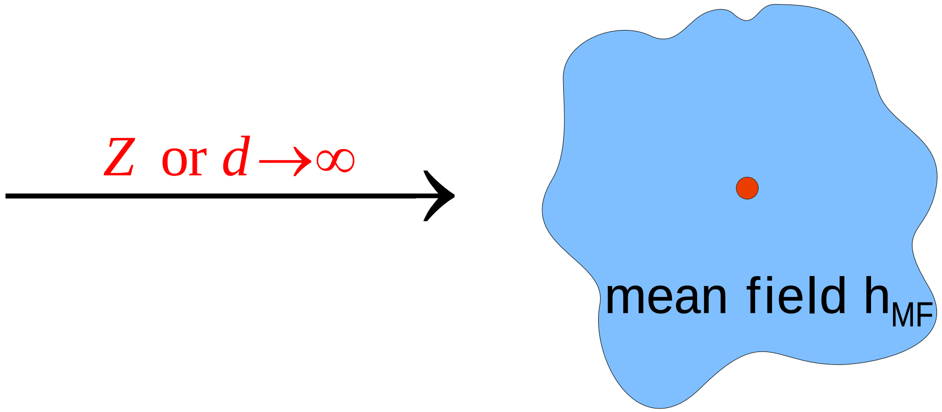
Interacting spins/particles on a lattice

Face-centered cubic lattice

Dimension d=3



Z=12



Local (single-site) mean-field theory

Example: Ising model

$$H = J \sum_{\langle i,j \rangle} S_i S_j$$

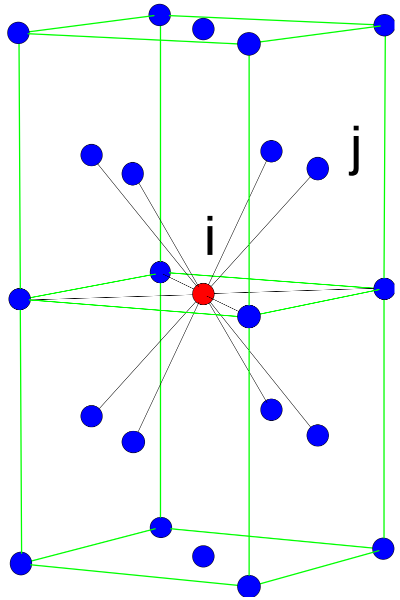
Simplest spin model

Exact sol. in d=1,2

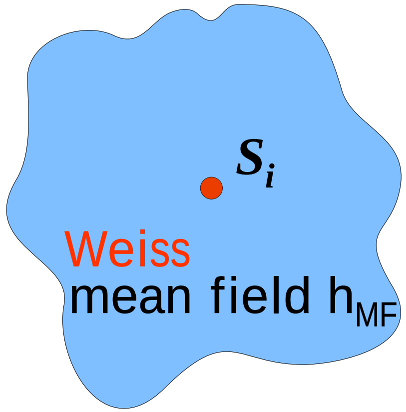
Best-known mean-field theory (MFT): Weiss MFT for the Ising model

$$H = J \sum_{\langle i,j \rangle} S_i S_j \xrightarrow{Z \text{ or } d \to \infty} H_{MF} = \underbrace{h_{MF}}_{J^* \langle S \rangle} \sum_i S_i$$

Classical rescaling $J = \dfrac{J^*}{Z}$



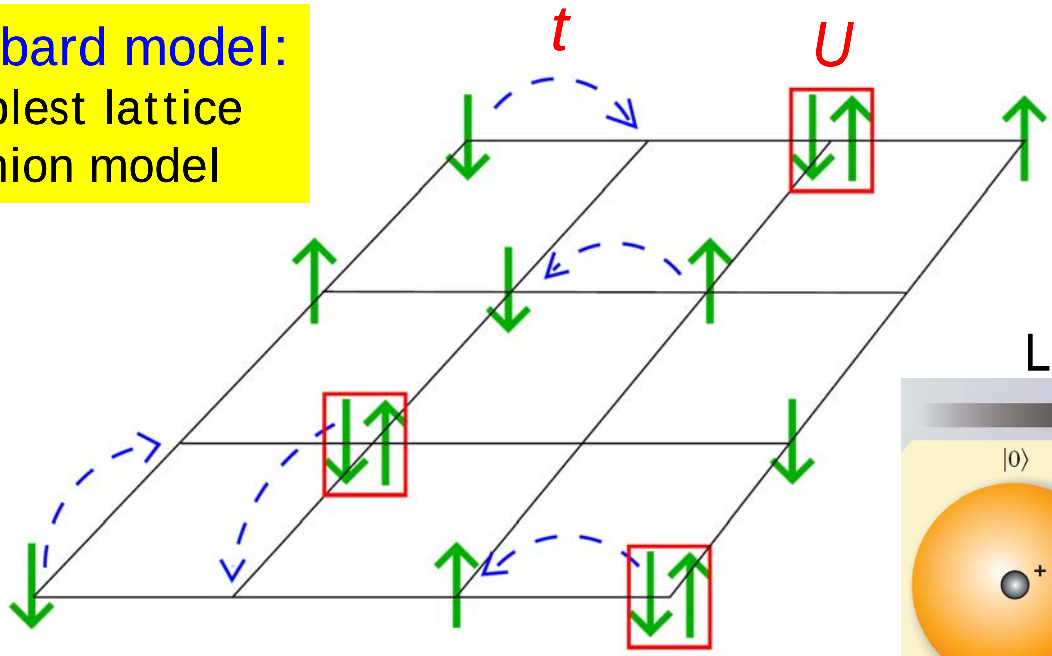
Z or $d \to \infty$



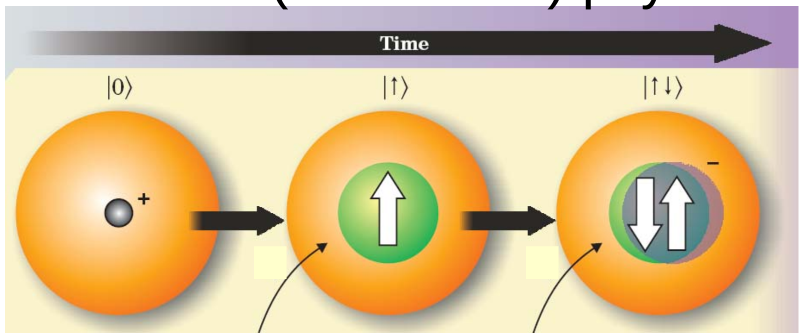
Local (single-site) mean-field theory

Conserving, thermodyn. consistent approximation, free of spurious singularities

Hubbard model:
Simplest lattice fermion model



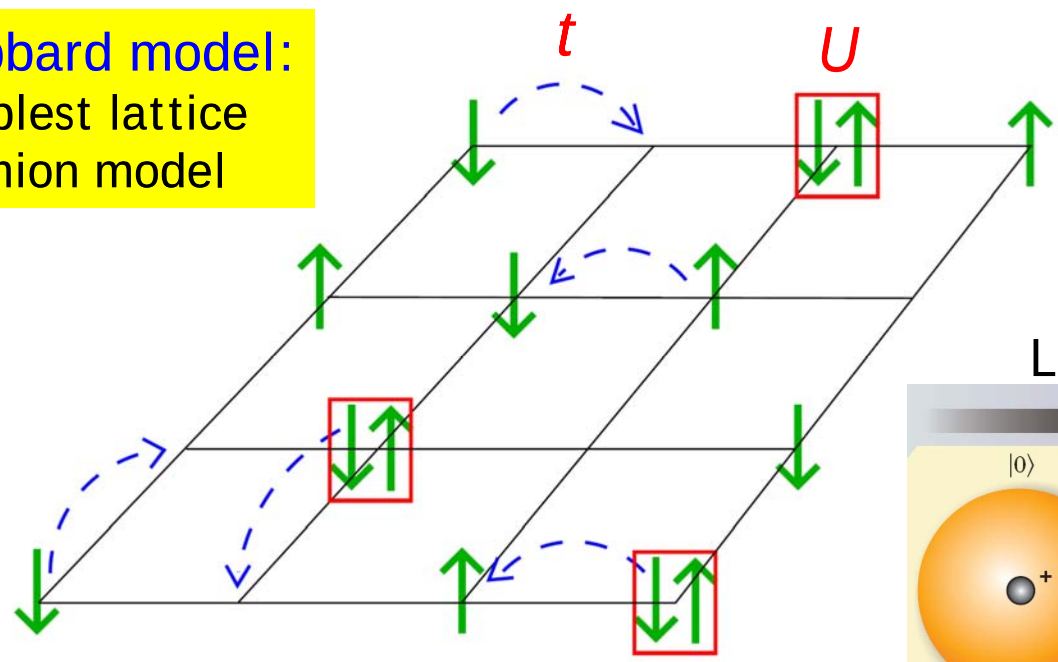
Local ("Hubbard") physics:



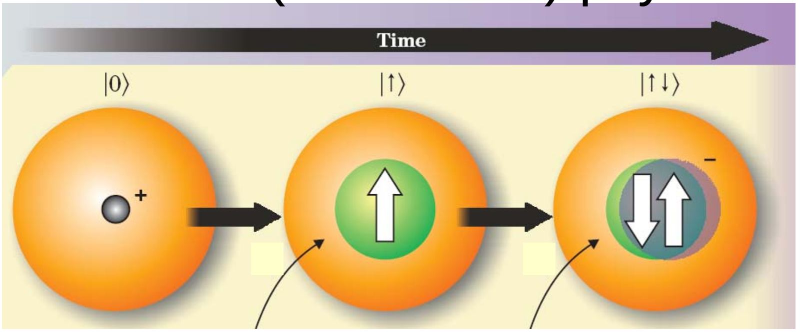
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Exact sol. in d=1

Hubbard model:
Simplest lattice fermion model



Local ("Hubbard") physics:



$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

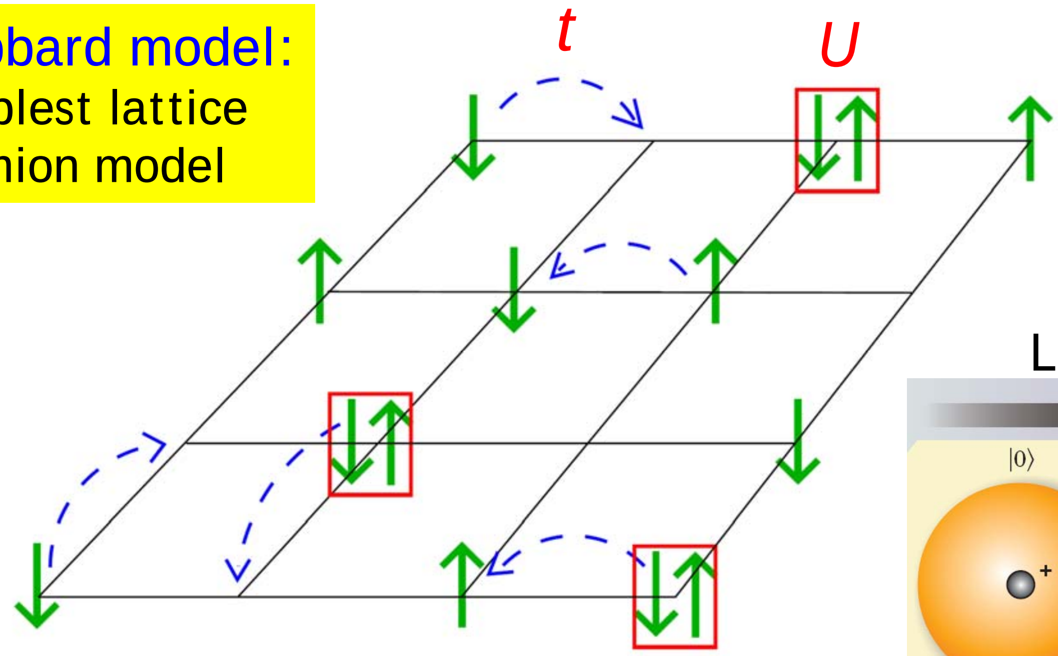
Analogy to Weiss MFT?

→ Hartree-(Fock) approx.

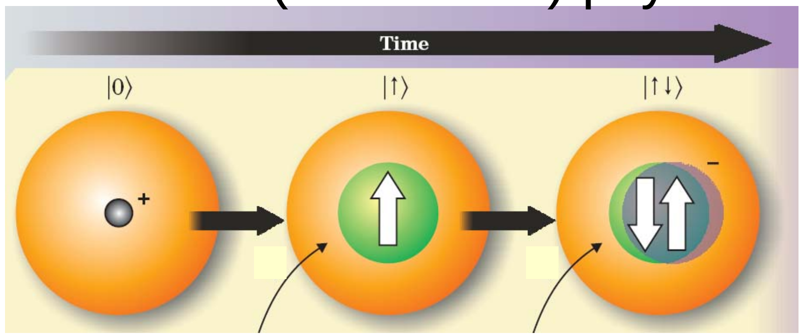
$$\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \rangle \approx \langle n_{\mathbf{i}\uparrow} \rangle \langle n_{\mathbf{i}\downarrow} \rangle$$

- Derivation of Weiss and Hartree MFTs
→ black board

Hubbard model:
Simplest lattice
fermion model



Local ("Hubbard") physics:



$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Z → ∞ limit?

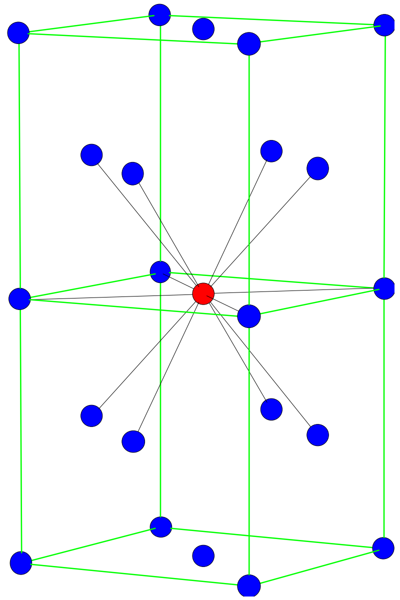
Hubbard model

$$H = -t \underbrace{\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma}}_{\text{non-local}} + U \underbrace{\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}}_{\text{local}} \xrightarrow{Z \text{ or } d \to \infty} ?$$

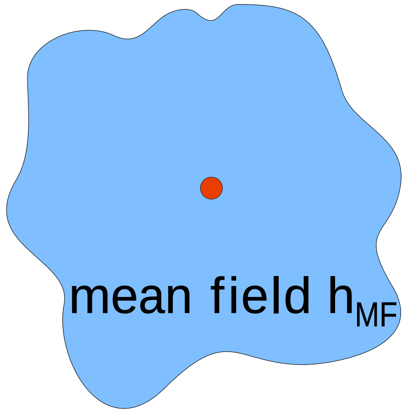
Simplifications?

Comprehensive MFT valid for all input parameters?

Scaling ?



$$\xrightarrow{Z \text{ or } d \to \infty}$$



?

Local (single-site) mean-field theory

Hubbard model

Metzner, DV (1989)

$$\langle H_{kin} \rangle_0 = -t \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \langle c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} \rangle_0$$

Amplitude for hopping j → NN i

$$\left| \text{Amplitude for hopping j} \rightarrow \text{NN i} \right|^2 = \text{Probability for hopping j} \rightarrow \text{NN i} = \frac{1}{Z}$$

Hubbard model

Metzner, DV (1989)

$$\langle H_{kin} \rangle_0 = \boxed{-t}_{\propto \frac{1}{\sqrt{Z}}} \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\langle c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle_0}_{\propto \frac{1}{\sqrt{Z}}}$$

Z or d$\to\infty$

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$

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Z or $d \to \infty$

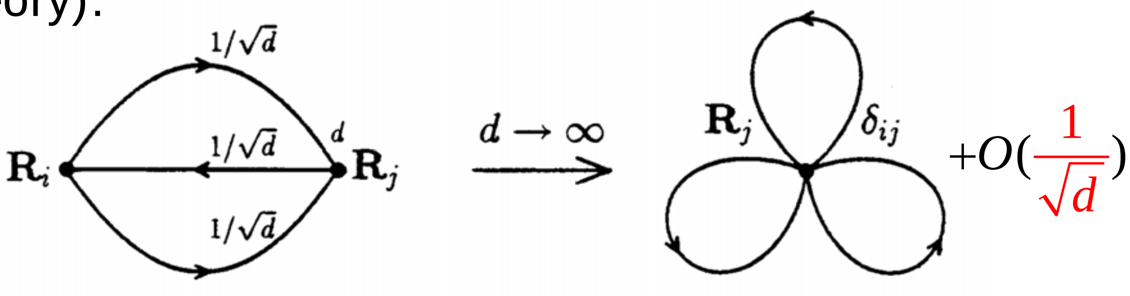
Quantum rescaling $t = \dfrac{t^*}{\sqrt{Z}}$

$\xrightarrow{Z \text{ or } d\to\infty}$ Collapse of all connected, irreducible diagrams in position space ("locality of perturbation theory")

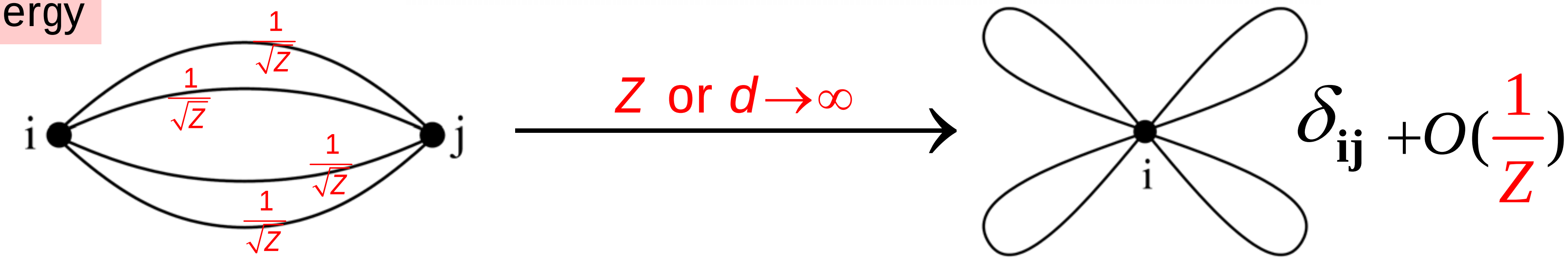
$\Rightarrow$ great simplifications

Examples (2. order pert. theory):

Self-energy



Energy



Hubbard model

Metzner, DV (1989)

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Z or d $\to \infty$

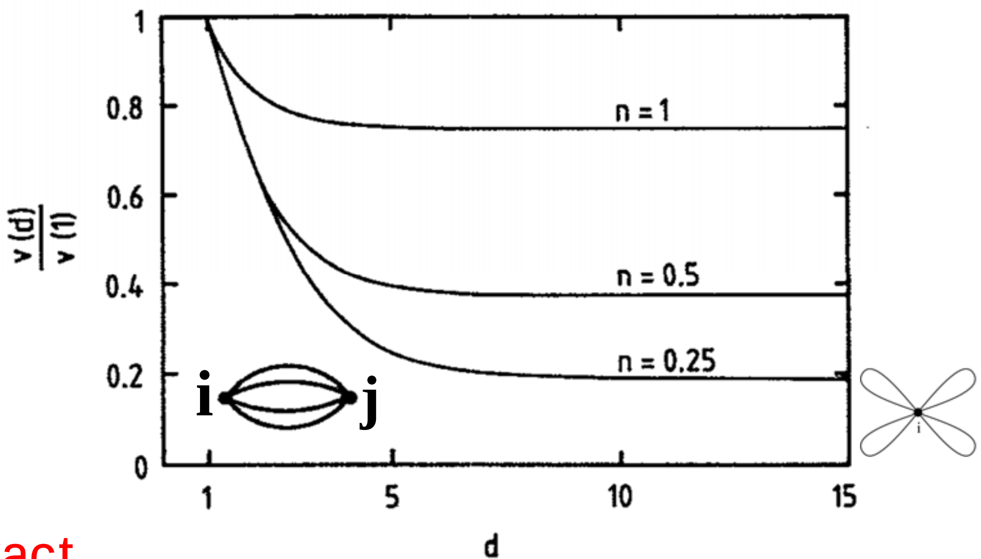
Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$

$\xrightarrow{Z \text{ or } d \to \infty}$ Collapse of all connected, irreducible diagrams in position space ("locality of perturbation theory")
$\Rightarrow$ great simplifications

Gutzwiller wave function

$$|\psi_G\rangle = e^{-\lambda \hat{D}} |\psi_0\rangle$$

d $\to \infty$: Gutzwiller (semi-classical) approximation becomes exact



Metzner, DV (1988)

Hubbard model

Metzner, DV (1989)

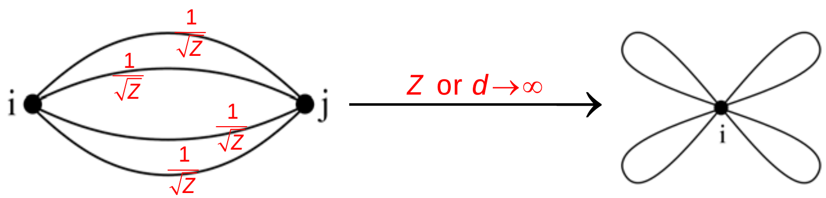
$$\langle H_{kin} \rangle_0 = -t \underbrace{\sum_{\mathbf{i},\sigma}}_{} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle_0}_{\propto \frac{1}{\sqrt{Z}}}$$

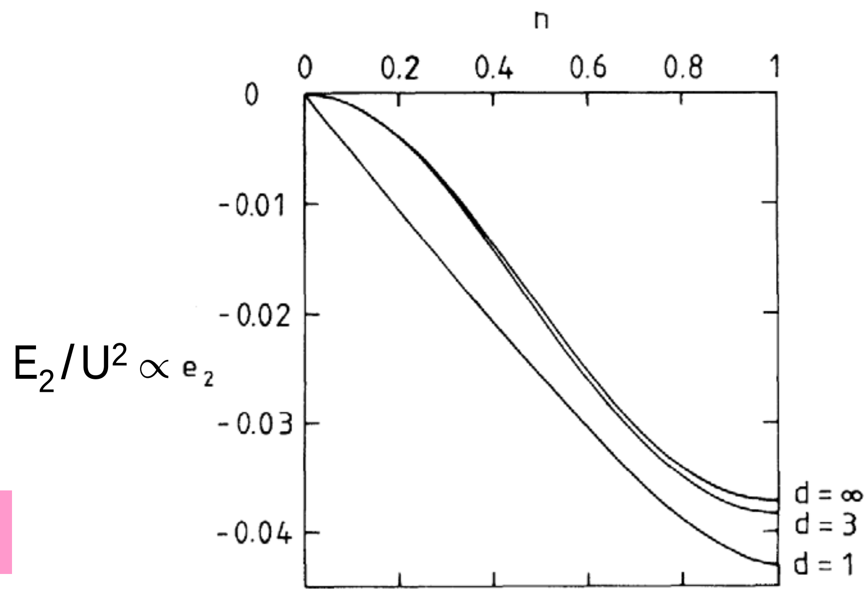
Z or d→∞ ; $-t \propto \frac{1}{\sqrt{Z}}$

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$

$\xrightarrow{Z \text{ or } d\to\infty}$ Collapse of all connected, irreducible diagrams in position space ("locality of perturbation theory")
⇒ great simplifications

E.g., correlation energy E_2





d=∞: excellent approximation for d=3

Hubbard model

Metzner, DV (1989)

$$\left\langle H_{kin} \right\rangle_0 = \underbrace{-t}_{\propto \frac{1}{\sqrt{Z}}} \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\left\langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \right\rangle_0}_{\propto \frac{1}{\sqrt{Z}}}$$

Z or d→ ∞

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$

$\xrightarrow{Z \text{ or } d \to \infty}$ Collapse of all connected, irreducible diagrams in position space ("locality of perturbation theory")

$\Rightarrow$ great simplifications

$$\Sigma_{ij}(\omega) \xrightarrow{d\to\infty} \Sigma_{ii}(\omega)\delta_{ij} \xrightarrow{FT} \Sigma_{\not{k}}(\omega)$$

Purely local self-energy: MFT!

Müller-Hartmann (1989)

Consequences of the *k*-independence of the self-energy

→ blackboard

Consequences of the *k*-independence of the self-energy

Propagator

$$G_{\vec{k}}(\omega) = \frac{1}{\omega - \epsilon_{\vec{k}} + E_F - \Sigma(\omega)}$$

Müller-Hartmann (1989)

Fermi surface is defined by $\omega = 0$

$$\boxed{\epsilon_{\vec{k}} + \Sigma_{\vec{k}}(0) = E_F}$$

Luttinger, Ward (1960):
Volume within Fermi surface is not changed by interactions →

$$\boxed{n = \sum_{\vec{k}\sigma} \theta[E_F - \epsilon_{\vec{k}} - \Sigma_{\vec{k}}(0)]}$$

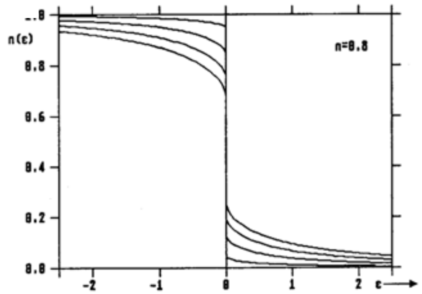
Effective mass

$$\frac{m^*}{m} = 1 - \left.\frac{d\Sigma}{d\omega}\right|_{\omega=0} = 1 + \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, \frac{Im\Sigma(\omega + i0^-)}{\omega^2} \geq 1$$

Momentum distribution

$$n_{\vec{k}} = \frac{1}{\pi}\int_{-\infty}^{0} d\omega\, ImG_{\vec{k}}(\omega)$$

Discontinuity at Fermi surface



$$n_{k_F^-} - n_{k_F^+} = (m^*/m)^{-1}$$ (Z-factor)

DOS: Fermi surface pinning

Hubbard model

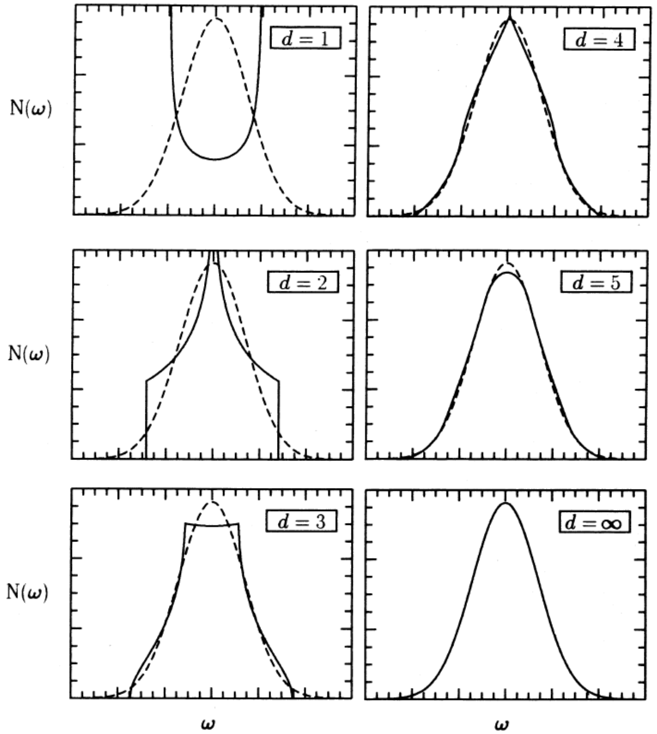
Metzner, DV (1989)

$$\langle H_{kin} \rangle_0 = -t \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\langle c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle_0}_{\propto \frac{1}{\sqrt{Z}}}$$

Z or d→ ∞ $\quad -t \propto \frac{1}{\sqrt{Z}}$

Quantum rescaling $\quad t = \frac{t^*}{\sqrt{Z}}$

Density of states for NN hopping on a hypercubic lattics



→ Training session

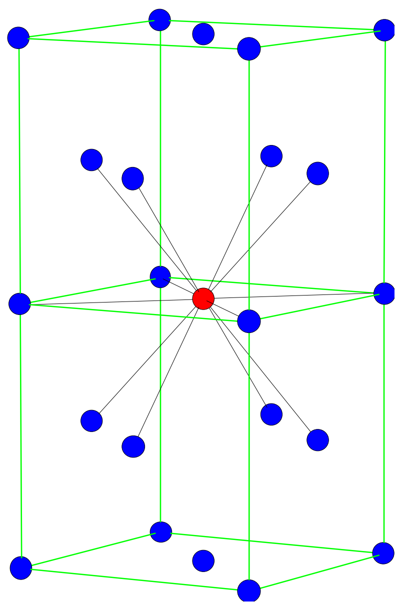
Gaussian
(normal distribution)

$d \to \infty$ mean-field theory: Hubbard model

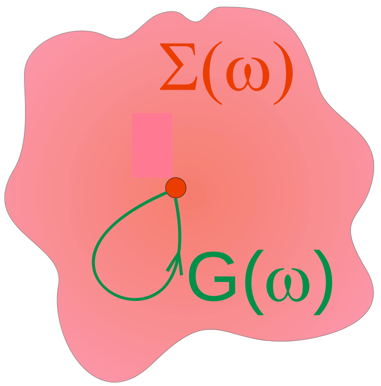
$$\langle H_{\text{kin}} \rangle = -\underbrace{t}_{\frac{1}{\sqrt{Z}}} \sum_{i\sigma} \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle}_{\frac{1}{\sqrt{Z}}}$$

Metzner, DV (1989)

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$


Z=12

Z or $d \to \infty$



Dynamical (single-site) mean-field theory

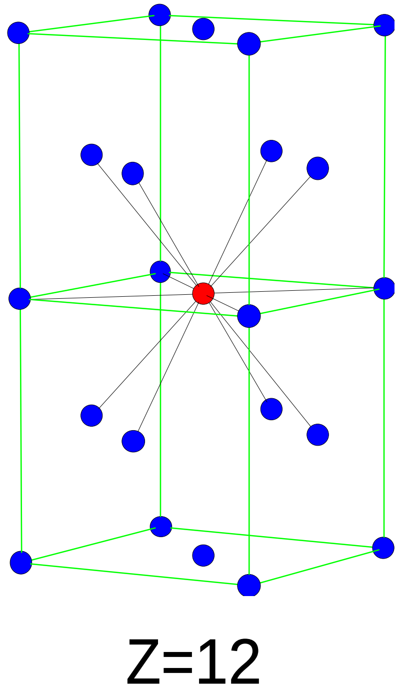
Müller-Hartmann (1989); Janis (1991)

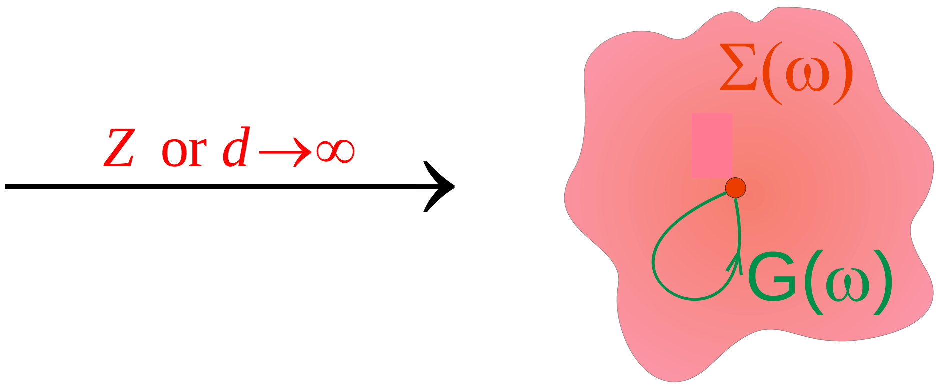
$d \to \infty$ mean-field theory: Hubbard model

$$\langle H_{\text{kin}} \rangle = -\underbrace{t}_{\frac{1}{\sqrt{Z}}} \sum_{i\sigma} \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle}_{\frac{1}{\sqrt{Z}}}$$

Metzner, DV (1989)

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$



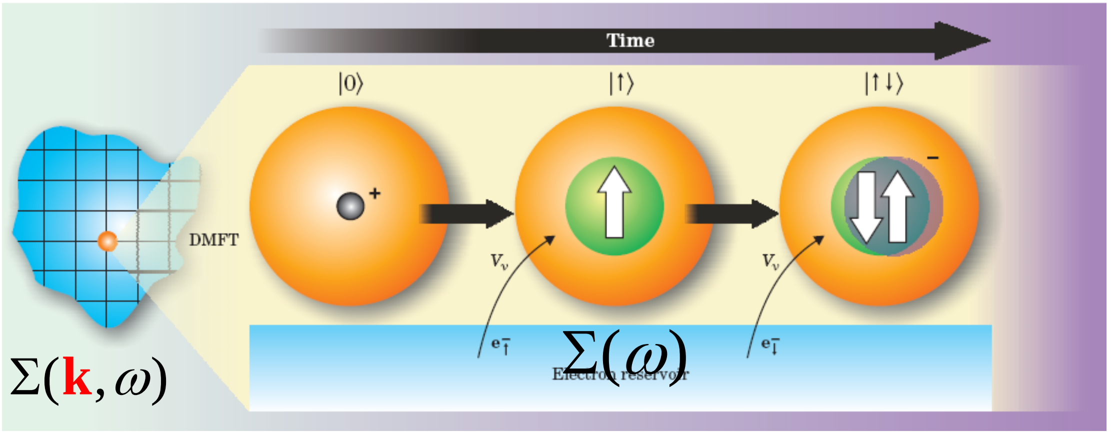


Single-impurity Anderson model
+ self-consistency

Georges and Kotliar (1992), Jarrell (1992)

Dynamical mean-field theory of correlated electrons

Proper time resolved treatment of local electronic interactions:



Kotliar, DV (2004)

DMFT: local theory with full many-body dynamics

→ Insights into

- Correlation phenomena at intermediate couplings
- Mott-Hubbard metal-insulator transition